

Carboxin

5234-68-4 | DTXSID0023951

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 314 °C

Global applicability domain: Inside

Local applicability domain index: 3.51e-01

Confidence level: 4.58e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Acetamidobiphenyl</div> <div>Measured: 355</div> <div>Predicted: 321</div>	<div>Image not found</div> <div>2-Acetylaminofluorene</div> <div>Measured: 303</div> <div>Predicted: 340</div>	<div>Image not found</div> <div>Propanil</div> <div>Measured: 351</div> <div>Predicted: 317</div>
<div>Image not found</div> <div>Ethyl oxanilate</div> <div>Measured: 280</div> <div>Predicted: 295</div>	<div>Image not found</div> <div>Phenacetin</div> <div>Measured: 244</div> <div>Predicted: 301</div>	